



AFRL-AFOSR-VA-TR-2016-0268

Multiscale Modeling and Characterization of the Effects of Damage Evolution
on the Multifunctional Properties of Polymer Nanocomposites

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07/27/2016
Final Report

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REPORT DOCUMENTATION PAGE				Form Approved OMB No. 0704-0188	
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1. REPORT DATE (DD-MM-YYYY) 13-07-2016		2. REPORT TYPE Final Report		3. DATES COVERED (From - To) From 15-04-2012 to 14-04-2016	
4. TITLE AND SUBTITLE Multiscale Modeling and Characterization of the Effects of Damage Evolution on the Multifunctional Properties of Polymer Nanocomposites				5a. CONTRACT NUMBER	
				5b. GRANT NUMBER FA9550-12-1-0205	
				5c. PROGRAM ELEMENT NUMBER	
6. AUTHOR(S) Gary D. Seidel				5d. PROJECT NUMBER	
				5e. TASK NUMBER	
				5f. WORK UNIT NUMBER	
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) VIRGINIA POLYTECHNIC INSTITUTE & STATE UNIVERSITY 300 TURNER ST NW, SUITE 4200 BLACKSBURG VA 24061-0001 (540) 231-5281				8. PERFORMING ORGANIZATION REPORT NUMBER	
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES) USAF, AFRL DUNS 143574726 AF OFFICE OF SCIENTIFIC RESEARCH 875 NORTH RANDOLPH STREET, RM 3112 ARLINGTON VA 22203				10. SPONSOR/MONITOR'S ACRONYM(S) AFOSR	
				11. SPONSOR/MONITOR'S REPORT NUMBER(S)	
12. DISTRIBUTION/AVAILABILITY STATEMENT Distribution A - Approved for Public Release					
13. SUPPLEMENTARY NOTES					
14. ABSTRACT The objective of the research was to develop a novel multiscale modeling approach for capturing the effects of damage evolution on the mechanical and electrical properties of carbon nanotube-polymer nanocomposites. Focus was placed on understanding and capturing the key deformation and damage mechanisms which lead to measurable changes in the macroscale sensing properties (e.g. changes in electrical conductivity or piezoresistivity) in proposed nanocomposite structural health monitoring sensors. As part of an addendum, the effort was extended to explore the use of carbon nanotube nanocomposite piezoresistive sensing in performing structural health monitoring in epoxy-based energetic materials. The focus was to distribute the sensing network throughout the epoxy matrix phase of mock energetic materials and assess whether or not the large nanocomposite gauge factors (2 – 20+, compared to the ~2 for conventional strain gauges) can be maintained within the energetic composite architecture.					
15. SUBJECT TERMS Carbon Nanotube, Nanocomposite, Structural Health Monitoring, Strain Sensing, Damage Sensing					
16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
a. REPORT	b. ABSTRACT	c. THIS PAGE			Gary D. Seidel
U	U	U	UU	9	19b. TELEPHONE NUMBER (Include area code) (540) 231-9897

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Final Performance Report

13 July 2016

for

Multiscale Modeling and Characterization of the Effects of Damage Evolution on the Multifunctional Properties of Polymer Nanocomposites

AFOSR Grant # FA9550-12-1-0205

Performance Period: 15 April 2012 to 14 April 2016

Gary D. Seidel

Aerospace and Ocean Engineering Department
Virginia Polytechnic Institute and State University

Includes Addendum:

Exploration of Structural Health Monitoring Capabilities of Carbon Nanotube-Epoxy
Nanocomposite Matrix in Epoxy-Based Energetic Materials

AFOSR Program Manager
Jennifer Jordan

(YIP) Multiscale Modeling and Characterization of the Effects of Damage Evolution on the Multifunctional Properties of Polymer Nanocomposites

Gary D. Seidel

Abstract

The objective of the research was to develop a novel multiscale modeling approach for capturing the effects of damage evolution on the mechanical and electrical properties of carbon nanotube-polymer nanocomposites. Focus was placed on understanding and capturing the key deformation and damage mechanisms which lead to measurable changes in the macroscale sensing properties (e.g. changes in electrical conductivity or piezoresistivity) in proposed nanocomposite structural health monitoring sensors. The effort centered on the development of a hybrid concurrent-hierarchical multiscale modeling approach for capturing the effects of the evolution of damage on the multifunctional properties of polymer nanocomposites. The novel multiscale approach encompassed both first principles atomistic modeling (Molecular Dynamics/Molecular Statics) and continuum level computational micromechanics modeling (Finite Element-based Asymptotic Expansion and Cohesive Zone Modeling) techniques in a hybrid concurrent-hierarchical scale bridging method. The research also included an experimental characterization component which provides both multiscale model input and model validation at multiple scales. The effort was divided into three focus areas: Atomistic Modeling of Nanoscale Interface Effects, Multiscale Continuum Micromechanics Modeling with Damage Evolution, and Nanocomposite Characterization for Model Validation. The objectives of each of these focus areas worked together to create a unified approach toward developing a validated multiscale model for capturing the effects of nanoscale damage evolution on the macroscale properties of carbon nanotube-polymer nanocomposites sensors.

As part of an addendum, the effort was extended to explore the use of carbon nanotube nanocomposite piezoresistive sensing in performing structural health monitoring in epoxy-based energetic materials. The focus was to distribute the sensing network throughout the epoxy matrix phase of mock energetic materials and assess whether or not the large nanocomposite gauge factors (2 – 20+, compared to the ~2 for conventional strain gauges) can be maintained within the energetic composite architecture. As a key to designing the embedded nanocomposite sensing and interpreting the sensor data is having a good material/constitutive model, novel multiscale modeling approaches for damage evolution and its impact on the multifunctional sensing properties were developed with emphasis on meshless methods for impact modeling such as peridynamics.

Summary

The grant was originally funded for three years as part of the Multi-Scale Structural Mechanics and Prognosis Program under Dr. David Stargel. The funding supported the efforts of two Ph.D. students and the PI for three years. The effort leveraged initial support for embedded structural health monitoring in composites as part of MURI-18 Synthesis Characterization and Modeling of Functionally Graded Hybrid Composites for Extreme Environments (contract/grant no.:FA-9550-09-0686) also under Dr. David Stargel which had support for one Ph.D. student. During year two of the grant, the project was transitioned to the Dynamic Materials and Interactions Program under

Dr. Jennifer Jordan. An addendum was added which provided funding for an additional student in year three and for a fourth year of funding for that student to begin exploring extensions of the grant activities towards meeting objectives of the DMI program. The total effort of both the original grant and addendum has resulted in 8 published journal publications ([1] [2] [3] [4] [5] [6] [7] [8]), with an additional publication still under review [9], and in 13 conference proceeding papers ([10] [11] [12] [13] [14] [15] [16] [17] [18] [19] [20] [21] [22]). The grant has partially supported the dissertation work of 4 Ph.D. students: Yumeng Li (completed Fall 2014), Adarsh Chaurasia (completed Spring 2016), Engin Sengezer (expected Spring 2017), and Naveen Prakash (expected Spring 2017). The addendum work has also supported the summer research activities of 1 undergraduate student: Stefan Povolny (completed BS Spring 2015, currently pursuing Ph.D.).

Year 1 activities focused developing interface models of load transfer between unfunctionalized carbon nanotubes and the surrounding polymer matrix, developing a model to incorporate the nanoscale effect of electron hopping between neighboring carbon nanotubes, and fabricating aligned carbon nanotube nanocomposite samples. MD simulations were performed to ascertain the traction-separation response of a representative unfunctionalized graphene/nanotube-polyethylene surface in response to both normal (mode I) and sliding (mode II) separations [2]. The traction-separation response was then used in finite element analysis of nanocomposite representative volume elements to assess the influence of the weak interface (compared to the infinitely stiff perfect interface typically assumed) on the effective elastic properties of the nanocomposite [2]. In parallel, a method was developed for incorporating the effects of electron hopping between carbon nanotubes in finite element analysis of nanocomposite representative volume elements [1] [11]. The approach was used to study the influence of volume fraction, barrier potential, and tension-compression loading on the effective electrical percolation and piezoresistive response of nanocomposites [1] [11]. Finally, carbon nanotubes were dispersed within a co-polymer precursor solution and aligned under AC electric field into filament structures which were then locked in place under photopolymerization curing [10]. The influence of varying AC field strength and frequency as well as exposure time on the resulting filament structure were assessed using optical microscopy and Raman spectroscopy, and the corresponding electrical conductivity of the cured samples was measured in both the alignment and transverse directions demonstrating electrical percolation in the alignment direction at a nanotube concentration well below the nominal electrical percolation concentration [10] [3].

Year 2 activities focused on extending the development of interface models of load transfer at the carbon nanotube-polymer interface to include varying degrees of functionalization, developing an electromechanical interface model to couple with the electron hopping model, and assessing the piezoresistive response of aligned carbon nanotube nanocomposite samples. MD simulations were again performed to ascertain the traction-separation response, but now of a representative functionalized graphene/nanotube-polyethylene surface in response to both normal (mode I) and sliding (mode II) separations [6]. The traction-separation response was then used in finite element analysis of nanocomposite representative volume elements to assess the influence of the functionalized interface on the effective elastic properties of the nanocomposite [6]. The influence of electron hopping through the carbon nanotube-polymer interface was incorporated into the finite element simulations of nanocomposite representative volume elements through the development of an electromechanically coupled cohesive zone model [12] [4], allowing for the assessment of interface damage on the effective piezoresistive strain and damage sensing response. Larger dog-

bone samples of nanocomposites with long range alignment and varying concentration of carbon nanotubes were fabricated and assessed in terms of their piezoresistive response in both the alignment and transverse to alignment directions [13].

Year 3 activities shifted the focus of interface models to consider functionalization in cross-linked polymer matrices, the assessment of sensing of damage accumulation under cyclic loading, the development of a concurrent multiscale approach, and efforts to measure damage detection in fabricated nanocomposite samples. Year three was also the first year of the addendum which focused on developing a meshless method tool for impact analysis. MD simulations were again performed to ascertain the traction-separation response, but now of representative unfunctionalized and functionalized graphene/nanotube-epoxy surfaces in response to both normal (mode I) and sliding (mode II) separations [13]. The traction-separation response was then used in finite element analysis of nanocomposite representative volume elements to assess the influence of the functionalized interface on the effective elastic properties of nanocomposite systems having cross-linked polymer networks [13]. Finite element simulations of nanocomposite representative volume element response with interface damage under cyclic loading were performed to assess the loading/unloading variation in effective gauge factor [14] [18] [9], and were compared to efforts assess the influence of matrix damage on the electron hopping mechanism of piezoresistivity [13]. Initial steps were also taken towards establishing a two-scale concurrent multiscale model within a finite element framework in which deformations are passed down from the macroscale to the subscales (corresponding to various material points at the macroscale) where local microstructure evolves and results in updated effective properties which are passed back up to the macroscale yielding a heterogeneous and evolving distribution of constitutive properties within the macroscale [5]. The approach was used to assess the effects of mesoscale distribution of carbon nanotube bundles on the effective piezoresistive response of polymer nanocomposite [5]. Efforts to assess damage detection in fabricated nanocomposite samples included the testing of aligned tensile samples to failure under cyclic loading and the exploration of the application of notched bending and compact tension samples for epoxy and elastomer matrices [13] [15] [16]. Finally, the exploration of a meshless method for assessing impact response of energetic materials with nanocomposite binders was initiated by exploring the application of bond-based peridynamics [17]. The initial focus was on extending bond-based peridynamics to capture a larger range of isotropic material response than those having a Poisson's ratio of 0.3 and on addressing the presence of sharp/distinct interfaces between fiber and matrix [17].

With the original grant having come to a close, year 4 activities focused solely on the objectives associated with the addendum. The year 4 activities included the extension of meshless impact analysis tool to include electromechanical coupling, on fabricating and testing a mock energetic material with a nanocomposite binder for its strain and damage sensing response, and on the application of a hierarchical multiscale model of the mock energetic material's strain and damage sensing response. Extension of peridynamics focused on including electromechanical response in general, which necessitated the simultaneous solution of momentum and electrostatic balance laws, in the context of variable resistance/constant resistivity interfaces, and in the context of electron hopping as a nonlocal effect [22] [7]. Once integrated, these efforts were applied towards assessing the dynamic piezoresistive response of a carbon nanotube-polymer nanocomposite bundle representative volume to an impulse load [22] [7]. Mock energetic material samples were fabricated consisting of sugar grains dispersed in epoxy with varying concentrations of carbon

nanotubes within the epoxy resulting in a nanocomposite binder [8] [21]. The mock energetic with nanocomposite binder was characterized with optical and scanning electron microscopy, and was assessed in terms of its piezoresistive response using dog-bone samples tested in tension to failure [8] [21]. Efforts to model the piezoresistive response of the nanocomposite bound mock energetic material took the form of finite element based simulations of representative volume elements consisting of a distribution of sugar grains bound to one another by electromechanical cohesive zones corresponding to the effective piezoresistive response of carbon nanotube-epoxy nanocomposites [8] [19] [20]. The simulations were used to assess the influence of carbon nanotube concentration, grain conductivity, grain interface-epoxy bond strength, and orientation of carbon nanotubes within the epoxy [8] [19] [20]. The simulations were also used to compare with experimental observation of the effective electromechanical response to provide an estimate of unknown experimental parameters, e.g. grain interface-epoxy bond strength [8].

Accomplishments

Key contributions included the assessment of load transfer at the nanoscale interface between carbon nanotubes and polymer matrices and its influence on the strain sensing and damage detection potential in nanocomposites, the demonstration of the potential strain and damage sensing of aligned carbon nanotube filament structures in nanocomposites, and an initial exploration of potential application of nanocomposite binders in energetic materials for structural health monitoring. Specific accomplishments include:

- Assessment of nanoscale interface load transfer between functionalized and unfunctionalized carbon nanotubes and thermoplastic and thermoset matrices revealed significant improvement in load transfer with increasing degree of functionalization, especially in the sliding mode.
- Development and application of electromechanical cohesive zones in nanoscale representative volume elements demonstrated the influence of the interface load transfer on the piezoresistive strain sensing, the ability to distinguish between strain sensing and damage detection, and the presence of a hysteretic-like response in loading and unloading piezoresistive response.
- Development and application of two-scale concurrent multiscale model demonstrated the importance of transitioning nanoscale electron hopping through the mesoscale distribution of carbon nanotube bundle network in increasing the gauge factor.
- Fabrication and characterization of nanocomposite samples have demonstrated the potential for strain and damage sensing. In particular, samples with aligned carbon nanotube filaments demonstrated good piezoresistive and higher electrical conductivity in the alignment direction, but even better piezoresistive response in the transverse direction. This is believed to be the result of the transverse direction being very near percolation and therefore percolating on the application of load due to Poisson's contraction.
- Development of electromechanically coupled peridynamics and its application to dynamic loading of carbon nanotube bundles indicates a consistent pulse-reflection response as tension/compression waves move through the representative volume element thus demonstrating the potential for detecting dynamic response.
- Fabrication and characterization of mock energetic sugar-epoxy nanocomposite samples demonstrated the potential for both strain sensing and damage detection in energetic materials.

- Initial modeling of the mock energetic materials using electromechanical cohesive zones further demonstrated the potential for strain sensing and damage detection through parametric study of carbon nanotube concentration and orientation distribution within the epoxy matrix, and provided an initial attempt at inverse estimation of sugar-epoxy nanocomposite properties which could not be measured directly experimentally.

Acknowledgement/Disclaimer

This work was sponsored by the Air Force Office of Scientific Research, USAF, under grant/contract number FA9550-12-1-0205. The views and conclusions contained herein are those of the authors and should not be interpreted as necessarily representing the official policies or endorsements, either expressed or implied, of the Air Force Office of Scientific Research or the U.S. Government.

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FA9550-12-1-0205

Principal Investigator Name

The full name of the principal investigator on the grant or contract.

Gary Don Seidel

Program Manager

The AFOSR Program Manager currently assigned to the award

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Reporting Period Start Date

04/15/2012

Reporting Period End Date

04/14/2016

Abstract

The objective of the research was to develop a novel multiscale modeling approach for capturing the effects of damage evolution on the mechanical and electrical properties of carbon nanotube-polymer nanocomposites. Focus was placed on understanding and capturing the key deformation and damage mechanisms which lead to measurable changes in the macroscale sensing properties (e.g. changes in electrical conductivity or piezoresistivity) in proposed nanocomposite structural health monitoring sensors. The effort centered on the development of a hybrid concurrent-hierarchical multiscale modeling approach for capturing the effects of the evolution of damage on the multifunctional properties of polymer nanocomposites. The novel multiscale approach encompassed both first principles atomistic modeling (Molecular Dynamics/Molecular Statics) and continuum level computational micromechanics modeling (Finite Element-based Asymptotic Expansion and Cohesive Zone Modeling) techniques in a hybrid concurrent-hierarchical scale bridging method. The research also included an experimental characterization component which provides both multiscale model input and model validation at multiple scales. The effort was divided into three focus areas: Atomistic Modeling of Nanoscale Interface Effects,

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A. K. Chaurasia and G. D. Seidel, "Computational micromechanics analysis of electron hopping induced conductive paths and associated macroscale piezoresistive response in carbon nanotube-polymer nanocomposites," Journal of Intelligent Material Systems and Structures, vol. 25, no. 17, pp. 2141-2164, 2014.

Y. Li and G. D. Seidel, "Multiscale Modeling of the Effects of Nanoscale Load Transfer on the Effective Elastic Properties of Unfunctionalized Carbon Nanotube-Polyethylene Nanocomposites," Modelling and Simulation in Materials Science and Engineering, vol. 22, p. 25023, 2014.

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X. Ren, A. K. Chaurasia, A. I. Oliva-Aviles, J. J. Ku-Herrera, G. D. Seidel and F. Aviles, "Modeling of mesoscale dispersion effect on the piezoresistivity of carbon nanotube-polymer nanocomposites via 3D computational multiscale micromechanics methods," Smart Materials and Structures, vol. 24, p. 065031, 2015.

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N. Prakash and G. D. Seidel, "Electromechanical peridynamics modeling of piezoresistive response of
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carbon nanotube nanocomposites," Computational Materials Science, vol. 113, pp. 154-170, 2016.

A. K. Chaurasia, E. C. Sengezer, K. K. Talamadupula, S. Povolny and G. D. Seidel, "Experimental Characterization and Computational Modeling of Deformation and Damage Sensing Through the Piezoresistive Response of Nanocomposite Bonded Surrogate Energetic Materials," Journal of Multifunctional Composites, vol. 2, no. 4, pp. 1-27, 2014.

A. Chaurasia and G. D. Seidel, "Computational Micromechanics Analysis of Electron Hopping and Interfacial Damage Induced Piezoresistive Response In Carbon Nanotube-Polymer Nanocomposites Subjected to Cyclic Loading Conditions," European Journal of Mechanics - A/Solids, In Review.

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A. Chaurasia and G. D. Seidel, "Computational Micromechanics Analysis of Electron Hopping Induced Piezoresistive Response in Carbon Nanotube-Polymer Nanocomposites," in 54th AIAA/ASME/ASCE/AHS/ASC Structures, Structural Dynamics and Materials Conference, Boston, Massachusetts, 2013.

A. Chaurasia, X. Ren and G. D. Seidel, "Computational Micromechanics Model to Study the Effective Macroscale Piezoresistivity of Carbon Nanotube-Polymer Nanocomposites for Strain and Damage Sensing," in Proceedings Paper for the ASME 2013 Conference on Smart Materials, Adaptive Structures and Intelligent Systems, Snowbird, Utah, 2013.

A. K. Chaurasia, X. Ren, Y. Li, E. C. Sengezer, J. Burton and G. D. Seidel, "Computational Modeling and Experimental Characterization of Macroscale Piezoresistivity in Aligned Carbon Nanotube and Fuzzy Fiber Nanocomposites," in 55th AIAA/ASME/ASCE/AHS/ASC Structures, Structural Dynamics and Materials Conference at AIAA SciTech 2014, National Harbor, Maryland, 2014.

A. K. Chaurasia and G. D. Seidel, "Sensing Interfacial Damage Initiation, Evolution and Accumulation in Carbon Nanotube-Polymer Nanocomposites Under Cyclic Loading: A Computational Micromechanics Approach," in Proceedings Paper for the 2014 Conference on Smart Materials, Adaptive Structures & Intelligent Systems (SMASIS), Newport, Rhode Island, USA, 2014.

E. Sengezer and G. Seidel, "Experimental Characterization of Damage Evolution in Carbon Nanotube-Polymer Nanocomposites," in Proceedings Paper for the 2014 Conference on Smart Materials, Adaptive Structures & Intelligent Systems (SMASIS), Newport, Rhode Island, USA, 2014.

E. Sengezer and G. Seidel, "Experimental Characterization of Damage Evolution in Carbon Nanotube-Polymer Nanocomposites," in Proceedings Paper for the 56th AIAA/ASME/ASCE/AHS/ASC Structures, Structural Dynamics and Materials Conference at AIAA SciTech 2015, Kissimmee, Florida, USA, 2015.

N. Prakash and G. Seidel, "A novel two-parameter linear elastic constitutive model for bond based peridynamics," in Proceedings Paper for the 56th AIAA/ASME/ASCE/AHS/ASC Structures, Structural Dynamics and Materials Conference at AIAA SciTech 2015, Kissimmee, Florida, USA, 2015.

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K. Talamadupula, A. Chaurasia and G. Seidel, "2-Scale Hierarchical Multiscale Modeling of Piezoresistive Response in Polymer Nanocomposite Bonded Explosives," in Proceedings Paper for the ASME 2015 Conference on Smart Materials, Adaptive Structures and Intelligent Systems in Session 2-8 Smart Materials for Sensing Stretch and Pressure, Colorado Springs, Colorado, USA, 2015.

A. Chaurasia and G. Seidel, "Multiscale Modeling of Effective Piezoresistivity in Nanocomposite Bonded Explosives," in Proceedings Paper for the 57th AIAA/ASME/ASCE/AHS/ASC Structures, Structural Dynamics and Materials Conference at AIAA SciTech 2016, San Diego, California, USA, 2016.

E. Sengezer, S. Povolny and G. Seidel, "Real Time In-Situ Sensing of Damage Evolution in Carbon Nanotube-Polymer Nanocomposite Bonded Surrogate Energetics," in Proceedings Paper for the 57th AIAA/ASME/ASCE/AHS/ASC Structures, Structural Dynamics and Materials Conference at AIAA SciTech 2016, San Diego, California, USA, 2016.

N. Prakash and G. Seidel, "A Coupled Electromechanical Peridynamics Framework for Modeling Carbon

Nanotube Reinforced Polymer Composites," in Proceedings Paper for the 57th AIAA/ASME/ASCE/AHS/ASC Structures, Structural Dynamics and Materials Conference at AIAA SciTech 2016, San Diego, California, USA, 2016.

2. New discoveries, inventions, or patent disclosures:

Do you have any discoveries, inventions, or patent disclosures to report for this period?

No

Please describe and include any notable dates

Do you plan to pursue a claim for personal or organizational intellectual property?

Changes in research objectives (if any):

None

Change in AFOSR Program Manager, if any:

Changed from Dr. David Stargel to Dr. Jennifer Jordan

Extensions granted or milestones slipped, if any:

None

AFOSR LRIR Number

LRIR Title

Reporting Period

Laboratory Task Manager

Program Officer

Research Objectives

Technical Summary

Funding Summary by Cost Category (by FY, \$K)

	Starting FY	FY+1	FY+2
Salary			
Equipment/Facilities			
Supplies			
Total			

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Appendix Documents

2. Thank You

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